PHYSICAL REVIEW B VOLUME 9, NUMBER 12 15 JUNE 1974

Momentum density and Compton profile of the inhomogeneous interacting electronic system. I. Formalism

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(Received 31 December 1973)

A general formalism to determine the momentum density and Compton profiles of an inhomogeneous interacting electron system is proposed. The method is based on Feynman's theorem and the Hohenberg-Kohn theory of the inhomogeneous electron gas. Functional-derivative techniques are used. The results emcompass many of the previous approaches as special cases and present them from a unified viewpoint. In addition, several new approximate methods for calculating the Compton profiles of electronic systems are proposed.

I. INTRODUCTION

The single-particle momentum density of an inhomogeneous electronic system (e.g., atoms, molecules, and solids) is a rather interesting and important quantity to study. Its importance rests on the fact that it can be measured, rather directly, by high-energy (x-ray or γ-ray) Compton-scattering experiments.[1] Its interest, in the context of condensed-matter physics, rests on the fact that it is a relatively simple function which incorporates, in a nontrivial way, the many-body aspects of the interactions between the constituents of the system. In particular, for metals, this function gives information about the shape of the Fermi surface[2,3] and the importance of short-range electron-electron and electron-ion collision. The momentum density provides us with an experimentally observed function of a single variable which may be used to compare approximate wave functions of the many-body system. Such a comparison may ultimately be useful in discriminating different sets of wave functions which yield equally good estimates, for example, of the ground-state energy.

In a typical experiment,[4,5] the energy spectrum of monochromatic x-rays scattered through 180° by a sample (i.e., the electronic system) is measured. Because of the high energy of the photons used and because of the high-recoil energy of the electrons relative to typical atomic energies, the so-called impulse approximation is applicable. In this case, the differential cross section is found to be linearly proportional to $J(q)$ where[1,3]

$$J(q) \equiv \int dp_x\, dp_y\, [N_{\vec{p}}]_{p_z=q} \quad , \tag{1.1}$$

function of the electronic system and $a_{\vec{p}}$, $a^{\dagger}_{\vec{p}}$ are, respectively, the annihilation and creation operators of the free-electron state

$$|p\rangle \equiv e^{i\vec{p}\cdot\vec{r}} \tag{1.3}$$

In (1.1) the z axis is chosen as the direction of $\vec{k}$, the momentum transfer, and q is given by

$$q = \tfrac{1}{2}k - m\omega/k \quad , \tag{1.4}$$

with ω being the energy transferred in the scattering event.

In this paper we assume that the impulse approximation is valid so that $J(q)$, the Compton profile, as defined in (1.1) gives us a two-component average of the three-dimensional momentum density $N_{\vec{p}}$. In what follows we attempt to find an effective way of calculating $N_{\vec{p}}$ and thus $J(q)$, taking both the intrinsic inhomogeneities and the Coulomb correlation between the electrons into account.

Previous efforts to understand the momentum density or the Compton profiles of electronic systems fall into either one of the following four categories.

(a) First calculate the wave functions of the many-electron system (e.g., in some sort of Hartree-Fock approximation for atoms,[6-8] self-consistent approximations for molecules,[9] and Wigner-Seitz approximations[10] or pseudo-wave-functions[11] for solids, etc.), and then Fourier transform the wave functions to obtain the momentum density. This is usually done by assuming that the wave function is an antisymmetrized product of single-particle wave functions and is thus strictly within

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(c) Confine oneself to the homogeneous case and treat the interelectron Coulomb interaction in the random-phase approximation (RPA)[13–15] and in some cases go beyond RPA to include some exchange effects.[16,17] The Compton profiles corresponding to these various approximate results of $N_{\vec{p}}$ are also available.[2,18]

(d) A full many-body treatment for conduction electrons in metals with weak crystal fields that include both the interelectron and electron-ion interactions.[18–20]

Our method of calculating the momentum density, or the Compton profile, of a general inhomogeneous interacting electronic system as presented in the following includes all the four categories of previous approach as special cases[21] and suggests several new approximate methods, one of which is applied to atomic systems in the following paper.[22] In Sec. II, the general formalism is presented, and several special cases are spelled out in Sec. III. Section IV concludes the paper.

II. FORMULATION

For simplicity of presentation the electronic system we consider here is nonrelativistic and at zero temperature. Because of the high Fermi temperature and low Fermi velocity (relative to the velocity of light) characterizing most simple materials these conditions are usually satisfied. The generalization to nonzero temperature presents no conceptual problems and is presented elsewhere.[2] The essence of our approach is a combination of Feynman's theorem[23] and the Hohenberg-Kohn formulation[24] of inhomogeneous electron gas. Our method of finding the momentum density of an inhomogeneous electron liquid described by the Hamiltonian H is based on the following two steps.[25]

A. Connection between momentum density and ground-state energy

Feynman's theorem[23] implies the relation

$$N_p = \left[\frac{\partial E_p(\lambda)}{\partial \lambda}\right]_{\lambda=0} , \tag{2.1}$$

where $E_p(\lambda)$ is the exact ground-state energy of $H_p(\lambda)$ and

$$H_p(\lambda) \equiv H + \lambda a_p^\dagger a_p . \tag{2.2}$$

Here $p = (\vec{p}, \sigma_p)$ denotes the momentum and spin of the plane-wave state of an electron. Thus, a knowledge of the ground state energy of a system with the modified Hamiltonian given in (2.2) enables one to calculate N_p. The question then is how to find suitable expressions for the ground-state energy of a complicated system in a realistic yet sufficiently general fashion so as to permit a variety of approximations. The Hohenberg-Kohn formulation[24] of this problem provides us with such a scheme.

B. Ground-state energy as a functional of electron density

For a system of nonrelativistic interacting electrons in an external potential $V(\vec{r})$ (the source of the inhomogeneity), the Hamiltonian has the form ($\hbar = e^2 = m = 1$)

$$H = T + U + V , \tag{2.3}$$

where

$$T = \tfrac{1}{2} \int \nabla\psi^\dagger(\vec{r})\, \nabla\psi(\vec{r})\, d\vec{r} , \tag{2.4}$$

$$U = \frac{1}{2} \int \frac{1}{|\vec{r} - \vec{r}\,'|} \psi^\dagger(\vec{r})\, \psi^\dagger(\vec{r}\,')\, \psi(\vec{r}\,')\, \psi(\vec{r})\, d\vec{r}\, d\vec{r}\,' , \tag{2.5}$$

$$V = \int V(\vec{r})\, \psi^\dagger(\vec{r})\, \psi(\vec{r})\, d\vec{r} . \tag{2.6}$$

$\psi(\vec{r})$ and $\psi^\dagger(\vec{r})$ are the mutually conjugate second-quantized field operators. When $\psi(\vec{r})$ is written in terms of the a_p's, the annihilation operators for plane-wave states, Eq. (2.4), become

$$T = \sum_k \epsilon_k a_k^\dagger a_k , \tag{2.7}$$

where

$$\epsilon_k \equiv \tfrac{1}{2} k^2 . \tag{2.8}$$

In this representation (2.2) is

$$H_p(\lambda) = T_p + U + V , \tag{2.9}$$

where

$$T_p \equiv \sum_k \epsilon_k(p)\, a_k^\dagger a_k \tag{2.10}$$

and

$$\epsilon_k(p) \equiv \epsilon_k + \lambda \delta_{p,k} . \tag{2.11}$$

A comparison between Eqs. (2.3) and (2.9) shows that $H_p(\lambda)$ is obtained from H by replacing ϵ_k by $\epsilon_k(p)$. As a result, if we replace everywhere ϵ_k by $\epsilon_k(p)$ in the ground-state energy E of H we will get $E_p(\lambda)$. If we then go on and differentiate $E_p(\lambda)$ with respect to λ and set $\lambda = 0$, we will by Eq. (2.1) obtain N_p. In general, this differentiation with respect to λ is very involved because ϵ_k usually appears in E in a very complicated form. However, as we will show shortly, some simplification using the results of Hohenberg and Kohn[24] are possible.

Defining $n(\vec{r})$ by

$$n(\vec{r}) \equiv \langle \Phi_0 | \psi^\dagger(\vec{r})\, \psi(\vec{r}) | \Phi_0 \rangle , \tag{2.12}$$

Hohenberg and Kohn have shown that[24] (a) the ground-state energy E of H is a unique (and universal) *functional* of $n(\vec{r})$ and (b) E is stationary with respect to the variation of $n(\vec{r})$.

Point (a) implies that we may write

$$E = E[n] \tag{2.13}$$

$$\equiv \int V(\vec{r}) n(\vec{r})\, d\vec{r} + \frac{1}{2}\int \frac{n(\vec{r})n(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\, d\vec{r}\, d\vec{r}\,' + G[n] \;. \tag{2.14}$$

Eq. (2.14) is a formal expression used to define the correlation functional $G[n]$. Since $n(\vec{r})$ depends on the ground-state wave function, it is obvious that $n(\vec{r})$ also has a dependence on ϵ_k. Let us assume that under the transformation

$$\epsilon_k \rightarrow \epsilon_k(p) \;, \tag{2.15}$$

we have

$$n(\vec{r}) \rightarrow n_\lambda(\vec{r}) \;, \tag{2.16}$$

and

$$G[n] \rightarrow G_\lambda[n_\lambda] \;. \tag{2.17}$$

The dependence on p in $n_\lambda(\vec{r})$ and $G_\lambda(n_\lambda)$ is understood. As pointed out above, under the transformation (2.15), E of (2.14) becomes $E_p(\lambda)$. There are two sources of λ dependence in $E_p(\lambda)$. The first is an explicit dependence coming from $G_\lambda(n_\lambda)$ outside of $n_\lambda(r)$. The second is the dependence contained in $n_\lambda(r)$. When we differentiate $E_p(\lambda)$ with respect to λ in order to obtain N_p we may neglect the second dependence because of the stationary property [see point (b)] of E any first-order changes in $n(\vec{r})$ do not affect E. Consequently,

$$\left[\frac{\partial E_p(\lambda)}{\partial \lambda}\right]_{\lambda=0} = \left[\frac{\partial G_\lambda[n]}{\partial \lambda}\right]_{\lambda=0} \;, \tag{2.18}$$

since $E[n] - G[n]$ has no explicit dependence on ϵ_k. Using (2.1), we see that

$$N_p = \frac{\delta G[n]}{\delta \epsilon_p} \;, \tag{2.19}$$

where the functional derivative on the right-hand side of (2.19) is understood to have the same meaning as that in (2.1) plus the implicit understanding that $n(r)$ everywhere is kept intact during the differentiation.

III. SPECIAL CASES

In general the exact form of $G[n]$ is unknown except in some exceptionally simple cases. For noninteracting electrons and for interacting electrons in the Hartree and Hartree-Fock approximations it is straightforward to show that Eq. (2.19) is equivalent to

$$N_p = \sum_{i=1}^{N} |\langle p | \Phi_i \rangle|^2 \;, \tag{3.1}$$

the Fourier transform of the one-electron orbital Φ_i.

When the external potential $V(\vec{r})$ is a constant (for example, in the case of the jellium model where the positive charge is assumed to be uniform), the charge density $n(\vec{r})$ is also a constant. The energy functional $G[n]$ in (2.14) is then simply the sum of kinetic, exchange, and correlation energies of a homogeneous interacting gas of constant density n, and the momentum density $N_{\vec{p}}$ [Eq. (2.19)] is isotropic. A discussion of the qualitative and quantitative behavior of the momentum density and the corresponding Compton profiles in this case has been presented elsewhere[18,2] and will not be repeated here.

Aside from these cases we must resort to some approximate scheme which allows one to explicitly compute the Compton profile. We consider three such approximation schemes. The first one simply yields, within the framework of this formulation, the perturbation results for a weakly inhomogeneous system. The second gives us a new type of Fermi-Thomas approximation for a system with slowly varying density, while the third presents an in-principle self-consistent scheme for utilizing the results of density calculations to obtain an approximate calculation of the Compton profile.

A. Gas of almost constant density

For a gas of almost constant density, i.e.,

$$n(\vec{r}) = n_0 + \tilde{n}(\vec{r}) \;, \tag{3.2}$$

with

$$\tilde{n}(\vec{r})/n_0 \ll 1 \tag{3.3}$$

and

$$\int \tilde{n}(\vec{r})\, d\vec{r} = 0 \;, \tag{3.4}$$

the energy functional $G[n]$ [in (2.14)] can formally be expanded to second order in $n(\vec{r})$ i.e.,

$$G[n] = G[n_0] + \int K(\vec{r}-\vec{r}\,')\tilde{n}(\vec{r})\tilde{n}(\vec{r}\,')\, d\vec{r}\, d\vec{r}\,' + \ldots \;, \tag{3.5}$$

where $G[n_0]$ is the energy functional of a homogeneous gas of constant density n_0, i.e., the exchange and correlation energy. By (2.19)

$$N_p = N_p^0 + \Delta N_p \;, \tag{3.6}$$

where N_p^0 is the momentum density of the homogeneous gas of density n_0 and

$$\Delta N_p \equiv \int \frac{\delta K(\vec{r}-\vec{r}\,')}{\delta \epsilon_p} \tilde{n}(\vec{r})\tilde{n}(\vec{r}\,')\, d\vec{r}\, d\vec{r}\,' \;. \tag{3.7}$$

Defining the Fourier transforms by

$$K(\vec{r}) \equiv \sum_{\vec{q}} K(\vec{q})\, e^{-i\vec{q}\cdot\vec{r}} \;, \tag{3.8}$$

etc., (3.7) becomes

$$\Delta N_p = \sum_{\vec{q}} \frac{\delta K(\vec{q})}{\delta \epsilon_p} |\tilde{n}(\vec{q})|^2 \;. \tag{3.9}$$

By perturbation theory, treating V in (2.3) to lowest order, it is easy to show that $\tilde{n}(\vec{q})$ can be related to the external potential $V(\vec{q})$ through the dielectric function $\vec{\epsilon}(\vec{q}, \omega)$ of the homogeneous gas (of density n_0). In fact

$$\tilde{n}(\vec{q}) = \frac{V(\vec{q})}{v_q}\left(1 - \frac{1}{\epsilon(\vec{q}, 0)}\right) , \tag{3.10}$$

where

$$\begin{aligned} v_q &\equiv 4\pi/q^2 , \quad q \neq 0 \\ &\equiv 0 , \qquad q = 0 . \end{aligned} \tag{3.11}$$

Similarly

$$K(\vec{q}) = \tfrac{1}{2} v_q [\vec{\epsilon}(\vec{q}, 0) - 1]^{-1} . \tag{3.12}$$

Substituting (3.10) and (3.12) into (3.9) we have

$$\Delta N_p = \frac{1}{2} \sum_{\vec{q}} \frac{1}{v_q} \left| \frac{V(\vec{q})}{\vec{\epsilon}(\vec{q}, 0)} \right|^2 \frac{\delta \vec{\epsilon}(\vec{q}, 0)}{\delta \epsilon_p} . \tag{3.13}$$

For a crystal, the variable $\vec{q}$ in (3.13) is restricted to the reciprocal lattice vectors only, and we recover the equations obtained previously for a weakly inhomogeneous electron gas.[2,26] Equation (3.13) has already been applied to simple metals.[18]

B. Locally averaged method

In many cases of interest the momentum density of a uniform gas is expected to vary slowly with the electron density n. Qualitatively we can understand this if we remember that the momentum density of a uniform system is almost completely fixed by the Fermi momentum p_F. Since $p_F \sim n^{1/3}$, i.e., is rather weakly dependent on density, we would hope that a slowly varying approximation would be valid even for rather rapidly varying density functions.

In order to obtain an expression for the momentum density, it is natural to write the energy functional $G[n]$ as

$$G[n] = \int g_{\vec{r}}[n] n(\vec{r})\, d\vec{r} \tag{3.14}$$

(in the manner of Hohenberg and Kohn[24]). For a system of electrons with slowly varying density the functional $g_{\vec{r}}[n]$ may be expanded about the point $\vec{r}$, i.e.,

$$\begin{aligned} g_{\vec{r}}[n] = g^0[n] - \tfrac{1}{2} \int K_{n(\vec{r})}(\vec{r}\,') \\ \times [n(\vec{r} + \tfrac{1}{2}\vec{r}\,') - n(\vec{r} - \tfrac{1}{2}\vec{r}\,')]^2 d\vec{r}\,' + \dots , \end{aligned} \tag{3.15}$$

where $g^0[n]$ is the sum of kinetic, exchange, and correlation energies per electron of a homogeneous gas of constant density $n(\vec{r})$ and

$$K_{n(\vec{r})}(\vec{r}\,') \equiv \sum_{\vec{q}} K_{\vec{r}}(\vec{q})\, e^{-i\vec{q}\cdot\vec{r}\,'} , \tag{3.16}$$

$$K_{\vec{r}}(\vec{q}) = \tfrac{1}{2} v_q / \epsilon_{n(\vec{r})}(\vec{q}) . \tag{3.17}$$

$\epsilon_{n(\vec{r})}(\vec{q})$ is the static dielectric constant of a homogeneous gas of density $n(\vec{r})$. By (2.19) and (3.14)–(3.17),

$$N_{\vec{p}} = \int N_p^0(n(\vec{r})) n(\vec{r})\, d^3r + \delta N_p , \tag{3.18}$$

where $N_p^0(n(\vec{r}))$ is the momentum density of a uniform electron liquid with local density $n(\vec{r})$ and

$$\begin{aligned} \delta N_p = -\frac{1}{2} \int \frac{\delta K_{n(\vec{r})}(\vec{r}\,')}{\delta \epsilon_p} [n(\vec{r} + \tfrac{1}{2}\vec{r}\,') - n(\vec{r} - \tfrac{1}{2}\vec{r}\,')]^2 \\ \times n(\vec{r})\, d\vec{r}\, d\vec{r}\,' . \end{aligned} \tag{3.19}$$

We note that the first term on the right-hand side of (3.14) is isotropic in $\vec{p}$ although $n(\vec{r})$ may be anisotropic in $\vec{r}$ space. The anisotropy of N_p in $\vec{p}$ space only comes from δN_p.

The spirit underlying the approximation in (3.14) is the same as that in the Thomas-Fermi gas. The important difference lies in the fact that $n(\vec{r})$ in (3.14) is the exact electron density (coming from the complete solution of the many-body problem including inhomogeneity and electron correlations) compared to the simple $n(\vec{r})$ used in the standard[12] Thomas-Fermi approximation. Furthermore, the local momentum density in (3.18), $N_p^0(n)$, is the fully interacting electron liquid result while the counter part in the Thomas-Fermi approximation is nothing but the free-electron Fermi distribution. These two distinctions will be shown[22] to lead to significant modifications in the Compton profiles.

C. Self-consistent approximation

In some real systems the electron density is neither nearly constant nor slowly varying, so that the two approximations discussed in Secs. III A and III B cannot be used for quantitative calculations. A simple alternative approximation scheme is useful.

It has been shown by Kohn and Sham[27] that it is possible, at least formally, to replace the many-electron problem of (2.14) by a set of self-consistent one-electron equations. This is accomplished by splitting the energy functional $G[n]$ into two parts

$$G[n] \equiv T[n] + E_{xc}[n] , \tag{3.20}$$

where $T[n]$ is the kinetic energy of a system of inhomogeneous noninteracting electrons with density $n(\vec{r})$ and $E_{xc}[n]$ is, by definition, the exchange and correlation energy of an interacting system with density $n(\vec{r})$. The set of one-electron equations obtained from such an assumed form for the energy functional are[27]

$$[p^2/2m + V_{eff}(\vec{r})]\, \psi_i(\vec{r}) = E_i\, \psi_i(\vec{r}) , \tag{3.21}$$

with

$$V_{eff}(\vec{r}) \equiv V(\vec{r}) + \int \frac{n(\vec{r}\,')}{|\vec{r} - \vec{r}\,'|} d\vec{r}\,' + V_{xc}(\vec{r}\,') , \tag{3.22}$$

$$V_{xc}(\vec{r}) \equiv \frac{\delta E_{xc}[n]}{\delta n(\vec{r})} \;, \tag{3.23}$$

$$n(\vec{r}) = \sum_{i=1}^{N} |\psi_i(\vec{r})|^2 \;. \tag{3.24}$$

Here N is the number of electrons. The ground-state energy E of the system, by (2.14), becomes

$$E = \sum_{i=1}^{N} E_i - \frac{1}{2}\int \frac{n(\vec{r})n(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}\,d\vec{r}\,d\vec{r}\,' + E_{xc}[n] - \int V_{xc}(\vec{r})n(\vec{r})\,d\vec{r} \;. \tag{3.25}$$

Equation (3.25) is exact and Eqs. (3.21)–(3.24) have to be solved self-consistently.

In analogy with the one-electron approximation, the momentum density N_p may be found by simply differentiating Eq. (3.25) with respect to its implicit dependence on ϵ_p [see Eq. (2.19)] making sure to keep $n(\vec{r})$ fixed as per the discussion preceding Eq. (2.19). The result is

$$N_p = \sum_{i=1}^{N} \frac{\delta E_i}{\delta \epsilon_p} + \frac{\delta E_{xc}[n]}{\delta \epsilon_p} - \int \frac{\delta V_{xc}(\vec{r})}{\delta \epsilon_p} n(\vec{r})\,d\vec{r} \;. \tag{3.26}$$

Equation (3.26) may be made more explicit if we use the fact that

$$\frac{\delta E_i}{\delta \epsilon_p} = |\langle p|\psi_i\rangle|^2 + \langle \psi_i | \frac{\delta V_{\text{eff}}}{\delta \epsilon_p} | \psi_i\rangle \tag{3.27}$$

$$= |\langle p|\psi_i\rangle|^2 + \langle \psi_i | \frac{\delta V_{xc}(\vec{r})}{\delta \epsilon_p} | \psi_i\rangle \;. \tag{3.28}$$

Putting (3.28) into (3.26) and using (3.24), we finally find that

$$N_p = \sum_{i=1}^{N} |\langle p|\psi_i\rangle|^2 + \frac{\delta E_{xc}[n]}{\delta \epsilon_p} \;. \tag{3.29}$$

Equation (3.29) is similar to Eq. (3.1), however, unlike (3.1) it is formally exact. When the states $|\psi_i\rangle$ are the actual one-electron states as in the Hartree-Fock approximation then [as in (3.1)] the second term on the right-hand side of Eq. (3.29) is missing. In this self-consistent scheme the states $|\psi_i\rangle$ do not represent the "actual" one-electron states of the system as in the case of the Hartree-Fock calculations, thus the existence of the second term on the right-hand side of (3.29). This term represents the corrections to the momentum distribution due to correlations between the states $|\psi_i\rangle$.

To be more specific, let us consider one particular form of approximation for $E_{xc}[n]$, i.e., the "local" approximation. We set

$$E_{xc}[n] = \int \epsilon_{xc}(n(\vec{r}))n(\vec{r})\,d\vec{r} \;, \tag{3.30}$$

where $\epsilon_{xc}(n)$ is the exchange and correlation energy per electron of a homogeneous electron gas of constant density n. Computations in this approximation have been carried out for atoms by Tong and Sham[28] and for sodium metal by Tong.[29] By the rule of Sec. II B and Eq. (3.30)

$$\frac{\delta E_{xc}}{\delta \epsilon_p} = \int \frac{\delta \epsilon_{xc}(n)}{\delta \epsilon_p} n(\vec{r})\,d\vec{r} \tag{3.31}$$

$$= \int [N_p^0(n(\vec{r})) - N_p^F(n(\vec{r}))]n(\vec{r})\,d\vec{r} \;, \tag{3.32}$$

where $N_p^0(n)$ is defined after (3.18) and $N_p^F(n)$ is the free-electron Fermi distribution.

Another intriguing problem in the theory of the Compton profiles of solids is the correct handling of the core-orthogonalization effects.[30] This difficulty arises because we have artificially divided the electrons in the solid into core and conduction electrons. Although the case of sodium metal[3,20] (and similar materials) has been successfully attacked by simple approximate methods, the general core-orthogonalization problem is still a difficult one. The method presented in this section offers a way to avoid this problem completely. By treating all the electrons on the same footing[31] and using (3.29) and (3.31), we can obtain the momentum density or equivalently the Compton profile directly for the whole system if we know the density $n(\vec{r})$ everywhere and have a suitable approximate form for the momentum density of the homogeneous gas.

IV. CONCLUSIONS

We have presented a general formalism which enables us (formally) to determine the momentum density and Compton profiles of homogeneous interacting electronic systems. This method is based on the use of Feynman's theorem and the Hohenberg-Kohn theory of the inhomogeneous electron gas. This formal solution shifts the problem of finding the momentum density directly to that of finding the ground-state energy of the inhomogeneous system (with a slightly modified Hamiltonian). In this form it is possible to take advantage of the many explicit results obtained by workers who were interested in the ground-state energy problem. Many of the conventional approaches and a few new ones are recovered when explicit forms for this ground-state energy are postulated.

ACKNOWLEDGMENTS

We thank P. Eisenberger, P. C. Hohenberg, and B. Y. Tong for many helpful discussions. This work was initiated when one of us (L. L.) was a resident visitor at Bell Laboratories, Murray Hill, from Columbia University.

*Work at City College supported in part by O. N. R. and A. R. O. D.

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